

Exact approaches to constrained submodular minimization problems

Modern Aspects of Submodularity workshop, Georgia Tech
March 19th-22nd, 2012

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Submodular minimization problems

f : submodular function defined on 2^N

poly time

- unconstrained minimization

$$\min_{S \subseteq N} f(S)$$

- minimization over

- distributive lattice
- parity family
(Goemans–Ramakrishnan '95)

NP-hard

- size-constrained minimization

$$\min_{S \subseteq N} f(S) \quad \text{s.t. } |S| = k$$

and other constrained problems

- partition (clustering) problem

$$\begin{aligned} \min \quad & \sum_{i=1}^k f(S_i) \\ \text{s.t.} \quad & \{S_1, \dots, S_k\} \text{ is a partition} \\ & \text{of } N \text{ (} S_i \text{ is nonempty)} \end{aligned}$$

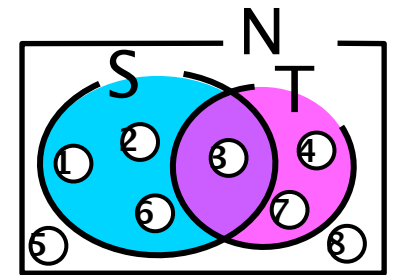
Zoya's talk

In this talk, we do not give approximation algorithms, but we give “exact” approaches to these NP-hard problems

Submodular function

- $N = \{1, \dots, n\}$ is a finite set
- A function f defined on $2^N = \{S : S \subseteq N\}$ is **submodular** if $\forall S, T \subseteq N$

$$f(S) + f(T) \geq f(S \cup T) + f(S \cap T)$$




- arises in many fields, e.g.,
graph theory, game theory, economics, **machine learning**

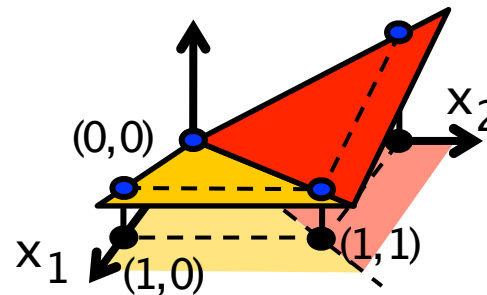
Applications of submodular functions are extensively studied in recent years

Submodular function

- **convex function** on $2^N \simeq \{0, 1\}^n$ ($N = \{1, 2, \dots, n\}$)

A submodular function f  The interpolation function \hat{f} is **convex**

$$\begin{aligned} f(\emptyset) &= 0 & f(\{1\}) &= 3 \\ f(\{2\}) &= 6 & f(\{1, 2\}) &= 3 \end{aligned}$$



The Lovász extension

- **unconstrained submodular function minimization**

$$\min f(S) \quad \text{s.t.} \quad S \subseteq N$$

Given a value-giving oracle

- ellipsoid method: Grötschel–Lovász–Schrijver (1981, 1988)
- combinatorial algorithm: Schrijver (2000), Iwata–Fleischer–Fujishige (2000)

• "practical" algorithm: Fujishige–Wolfe algorithm (Fujishige '91, '05)

↖ **standard algorithm in ML**

Examples of submodular functions

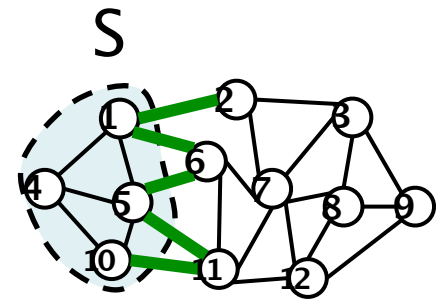
Graph $G = (N, E)$ with edge weights $w_e \geq 0$ ($e \in E$)

$\nwarrow N = \{1, \dots, n\}$

➤ Ex. 1. **Cut function** $C: 2^N \rightarrow \mathbb{R}$

$$C(S) = \sum \left\{ w_e : \begin{array}{l} e \in E \text{ has one endpoint in } S \\ \text{and one in } N-S \end{array} \right\}$$

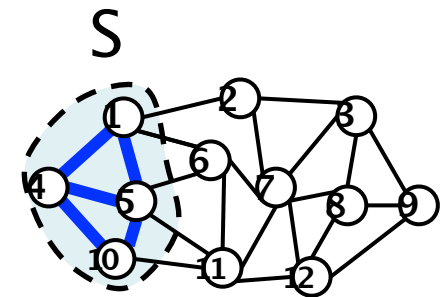
$\nwarrow C$ is **submodular**



➤ Ex. 2. **Edge intensity function** $I: 2^N \rightarrow \mathbb{R}$

$$I(S) = \sum \left\{ w_e : \begin{array}{l} \text{both of two endpoints} \\ \text{of } e \in E \text{ are in } S \end{array} \right\}$$

$\nwarrow -I$ is **submodular** (i.e. I is **supermodular**)



Constrained submodular minimization

In many cases, constrained submodular minimization problems are hard (cf. Talks of Jan Vondrak on Monday)

In this talk, we give

- Exact approach to **size-constrained submodular minimization (SSM)**
Nagano-Kawahara-Aihara, ICML '11

$$\begin{array}{ll} \min & f(S) \\ \text{s.t.} & |S| = k, \quad S \subseteq N \end{array}$$

➡ We use the minimum norm point of the base polyhedron

- Exact approach to **partition problem with submodular objective function**
Nagano-Kawahara-Iwata, NIPS '10

$$\begin{array}{ll} \min & \sum_{i=1}^k f(S_i) \\ \text{s.t.} & \{S_1, \dots, S_k\} \text{ is a} \\ & \text{partition of } N \text{ } (S_i \\ & \text{is nonempty}) \end{array}$$

➡ We use the theory of intersecting submodular functions

↖ We regard this problem as a clustering problem

OUTLINE

- Introduction
- Exact approach to size-constrained submodular minimization (Nagano-Kawahara-Aihara, ICML'11)
 - Example: Densest subgraph problem
 - Size-constrained submodular minimization (**SSM**)
 - The algorithm through the minimum norm base
- Exact approach to clustering problems with submodular objective functions (Nagano-Kawahara-Iwata, NIPS'10)
 - Example: Clustering of a network (minimum k-cut)
 - Minimum Average Cost (MAC) clustering
 - The algorithm using the Dilworth truncation
- Remarks

OUTLINE

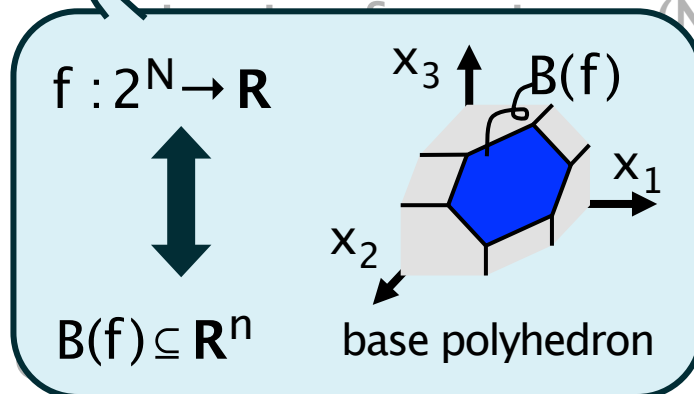
Exact approaches to constrained submodular minimization problems

- Introduction

- Exact approach to size-constrained submodular minimization (Nagano-Kawahara-Aihara, ICML '11)

- Example: Densest subgraph problem
- Size-constrained submodular minimization (**SSM**)
- The algorithm through the minimum norm base

- Exact approach to cluster



$$\min f(S)$$

$$\text{sub. to } S \subseteq \{1, \dots, n\}, |S| = k$$

This problem generalizes

- densest k-subgraph problem
- size-constrained minimum cut problem

Fundamental NP-hard problems

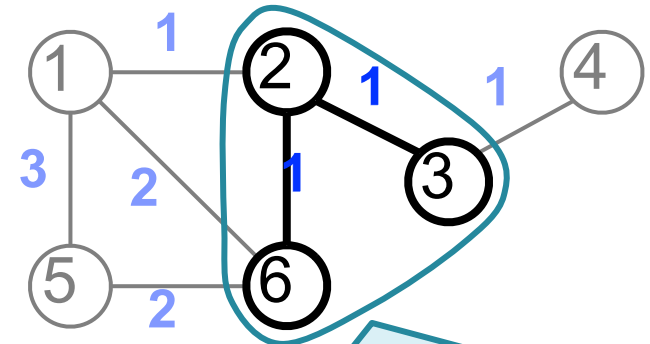
Example of **SSM**: Finding a dense graph

$G = (N, E)$: undirected graph

$\left\{ \begin{array}{l} \text{node set } N = \{1, \dots, n\} \\ \text{edge set } E \end{array} \right.$

Edge weights $w_e \geq 0 (e \in E)$

Integer k ($0 \leq k \leq n$)



$S = \{2, 3, 6\}$

$\Rightarrow I(\{2, 3, 6\}) = 1 + 1 = 2$

Densest k -subgraph problem:

Find a k -subset $S \subseteq N$ ($|S| = k$) that maximizes $I(S)$, where $I(S)$ is sum of **weights** of edges within S

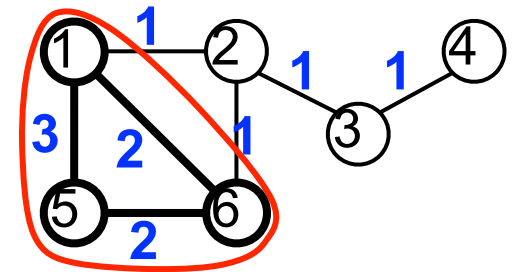
The set function $I: 2^N \rightarrow \mathbf{R}$ is supermodular ($-I$ is submodular)

Example of **SSM**: Finding a dense graph

Densest k -subgraph problem:

maximize $I(S)$

subject to $S \subseteq \{1, \dots, n\}$, $|S| = \underline{k}$



If $k=3$, an optimal solution is $\{1, 5, 6\}$

- NP-hard and constant factor approx algorithms are not known

Applications:

- Community detection problem in complex networks
- Identification of functional modules in protein-protein interaction networks

We deal with **a more general optimization problem**

size-constrained submodular minimization

Unconstrained submodular minimization (**USM**)

Problem (**USM**)

$$\begin{array}{ll} \min & f(S) \\ \text{s. t.} & S \subseteq N = \{1, \dots, n\} \end{array}$$

solvable in
poly time

➤ polynomial time:

ellipsoid method: Grotschel–Lovasz–Schrijver (1981, 1988)

combinatorial algorithm: Schrijver (2000), Iwata+ (2001)

➤ "**practical**": Fujishige–Wolfe algorithm (Fujishige '91, '05)

- **much faster in practice** (Fujishige+ 2006)

- this algorithm computes the **minimum norm base**

minimum L_2 -norm point in the **base polyhedron** $B(f) \subseteq \mathbb{R}^n$

- min norm base $\mathbf{x}^* \in \mathbb{R}^n \quad \Rightarrow \quad \text{minimizer of } f \subseteq \{1, \dots, n\}$

Size-constrained submodular minimization (**SSM**)

Problem (SSM)

$$\min f(S)$$

$$\text{s. t. } S \subseteq N, |S| = k$$

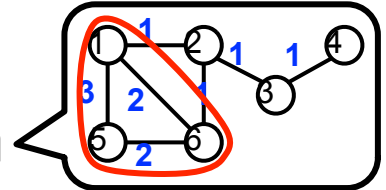
integer k ($0 \leq k \leq n$)

NP-hard

➤ There is no constant factor approximation algorithm that runs in polynomial time (Svitkina & Fleischer, '08 & '11)

➤ **special cases**

- $f = -|$ \Rightarrow Densest k -subgraph problem
- $f = C$ \Rightarrow Size-constrained minimum cut problem



Both of these are fundamental NP-hard problems

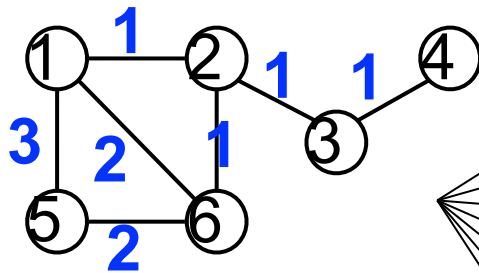
We propose an new method for (**SSM**) that

- uses the **minimum norm base**
- computes "**a portion of exact optimal solutions**"

Example of outputs of the proposed method

For all $k = 0, \dots, n$, consider the densest k -subgraph problems

$$\max I(S) \quad \text{s.t. } S \subseteq N, |S| = k$$



$$\max I(S) \text{ s.t. } S \subseteq N, |S| = 0$$

$$\max I(S) \text{ s.t. } S \subseteq N, |S| = 1$$

$$\max I(S) \text{ s.t. } S \subseteq N, |S| = 2$$

$$\max I(S) \text{ s.t. } S \subseteq N, |S| = 3$$

$$\max I(S) \text{ s.t. } S \subseteq N, |S| = 4$$

$$\max I(S) \text{ s.t. } S \subseteq N, |S| = 5$$

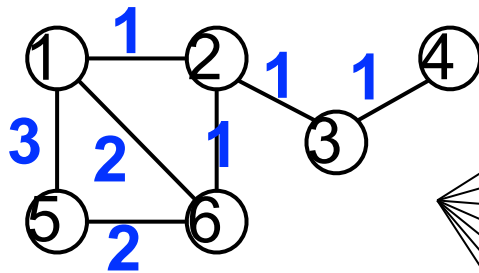
$$\max I(S) \text{ s.t. } S \subseteq N, |S| = 6$$

$n+1$ optimization problems

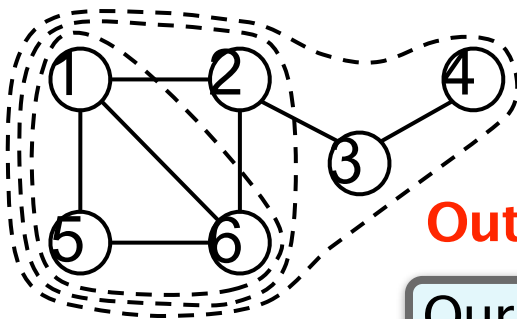
Example of outputs of the proposed method

For all $k = 0, \dots, n$, consider the densest k -subgraph problems

$$\max I(S) \quad \text{s.t. } S \subseteq N, |S| = k$$



proposed
method



Outputs: $\{\}, \{1, 5, 6\}, \{1, 2, 5, 6\}, \{1, 2, 3, 4, 5, 6\}$

$\max I(S) \text{ s.t. } S \subseteq N, |S| = 0$

→ **yes**

$\max I(S) \text{ s.t. } S \subseteq N, |S| = 1$

→ no

$\max I(S) \text{ s.t. } S \subseteq N, |S| = 2$

→ no

$\max I(S) \text{ s.t. } S \subseteq N, |S| = 3$

→ **yes**

$\max I(S) \text{ s.t. } S \subseteq N, |S| = 4$

→ **yes**

$\max I(S) \text{ s.t. } S \subseteq N, |S| = 5$

→ no

$\max I(S) \text{ s.t. } S \subseteq N, |S| = 6$

→ **yes**

Our method gives optimal solutions for $k = 0, 3, 4, 6$

Problem (**SSM**) in Machine Learning

$$\begin{array}{ll} \min & f(S) \\ \text{s.t.} & S \subseteq N, |S| = k \end{array}$$

■ Densest k-subgraph problem ($f = -l$)

- This problem naturally formulates a **community detection** problem in complex networks
- The identification of functional modules in **protein-protein interaction networks** is known as an important application (Dittrich et al., 2008)

■ Size-constrained minimum cut problem ($f = C$)

- This problem deals with an **explicit size constraint**
Contrastingly, **spectral clustering**, which is one of the most popular clustering algorithms, can deal with a minimum cut problem with an **implicit size constraint**

Definition: Base polyhedron

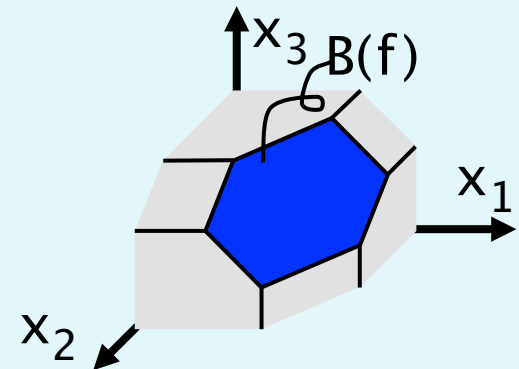
For a submodular function $f : 2^N \rightarrow \mathbf{R}$ with $f(\{\}) = 0$, the **base polyhedron** $B(f) \subseteq \mathbf{R}^n$ is given by

$$B(f) = \{ \mathbf{x} \in \mathbf{R}^n : \sum_{i \in S} x_i \leq f(S) \ (\forall S \subseteq N), \quad \sum_{i \in N} x_i = f(N) \}$$

$B(f)$ is determined by $2^n - 2$ inequalities and 1 equality

If $n = 3$, $B(f)$ is determined by

$$\begin{array}{ll} x_1 \leq f(\{1\}), & x_1 + x_2 \leq f(\{1,2\}) \\ x_2 \leq f(\{2\}), & x_1 + x_3 \leq f(\{1,3\}) \\ x_3 \leq f(\{3\}), & x_2 + x_3 \leq f(\{2,3\}) \end{array} \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} \begin{array}{l} 2^3 - 2 \text{ ineq} \\ 1 \text{ equality} \end{array}$$
$$x_1 + x_2 + x_3 = f(\{1,2,3\})$$



Minimum norm base and algorithms

The **minimum norm base** $\mathbf{x}^* \in \mathbf{R}^n$ is an optimal solution to

$$\min \sum_{i \in N} x_i^2 \quad \text{s. t.} \quad \mathbf{x} \in B(f)$$

- \mathbf{x}^* can be computed efficiently (Fujishige'80; Fleischer–Iwata'03, Nagano'07)
- Fujishige–Wolfe algorithm ('91, '05) finds \mathbf{x}^* **much faster in practice**

Algorithms through minimum norm base $\mathbf{x}^* \in \mathbf{R}^n$

■ The Fujishige–Wolfe algorithm for (USM) $\min f(S) \text{ s.t. } S \subseteq N$

$S^* = \{i \in N : x_i^* < 0\}$ minimizes f \Rightarrow The problem can be solved

In FW algorithm, we use **partial information** about \mathbf{x}^*

■ The **proposed algorithm** for (SSM) $\min f(S) \text{ s.t. } S \subseteq N, |S| = k$

In our algorithm, we use **full information** about \mathbf{x}^*

Algorithm for (SSM)

$$\min f(S) \text{ s.t. } S \subseteq N, |S| = k$$

Consider the following algorithm:

surprisingly simple!

Algorithm SSM

Step1: Compute the minimum norm base $\mathbf{x}^* \in B(f) \subseteq \mathbb{R}^n$

Step2: Let $\xi_1 < \xi_2 < \dots < \xi_d$ be distinct values of \mathbf{x}^*

Return $T_0 := \emptyset$ and $T_j := \{i \in V : x_i \leq \xi_j^*\}, \forall j = 1, \dots, d$

Example

The densest k -subgraph problems on  $\Rightarrow B(-I) \subseteq \mathbb{R}^6$

The minimum norm base is $\mathbf{x}^* = (-\frac{7}{3}, -2, -1, -1, -\frac{7}{3}, \frac{7}{3}) \in B(-I)$

Thus we have $\xi_1 = -\frac{7}{3}, \xi_2 = -2, \xi_3 = -1,$

$T_0 = \emptyset, T_1 = \{1, 5, 6\}, T_2 = \{1, 2, 5, 6\}, T_3 = \{1, 2, 3, 4, 5, 6\}$

optimal solutions for some of size constraints

Algorithm for (SSM)

$$\min f(S) \text{ s.t. } S \subseteq V, |S| = k$$

Consider the following algorithm:

surprisingly simple!

Algorithm SSM

Step1: Compute the minimum norm base $\mathbf{x}^* \in B(f) \subseteq \mathbb{R}^n$

Step2: Let $\xi_1 < \xi_2 < \dots < \xi_d$ be distinct values of \mathbf{x}^*

Return $T_0 := \emptyset$ and $T_j := \{i \in V : x_i \leq \xi_j^*\}, \forall j = 1, \dots, d$

Theorem [This work] For each $j \in \{0, 1, \dots, d\}$, $T_j \subseteq N$ is an optimal solution to Problem (SSM) w.r.t. $k = |T_j|$.

Algorithm SSM computes "a portion of exact optimal solutions"

Running time = computation of the minimum norm base

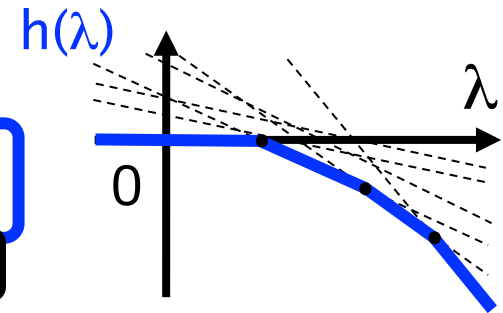
E.g., an implementation of the Fujishige–Wolfe algorithm can be found in a toolbox for submodular function optimization by Krause (2010, JMLR)

Proof of the validity of the algorithm **SSM**

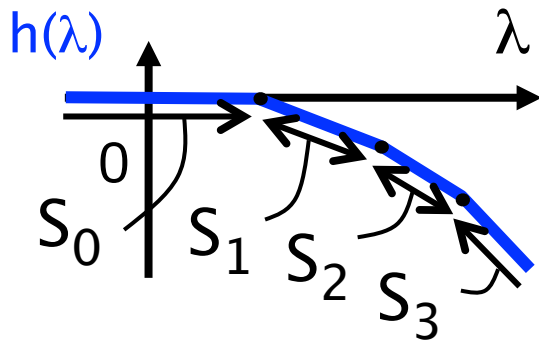
Define a function $h: \mathbf{R} \rightarrow \mathbf{R}$ as

$$h(\lambda) = \min\{f(S) - |S|\lambda : S \subseteq N\} \quad (\lambda \in \mathbf{R})$$

linear function in λ



h is the minimum of 2^n linear functions



Each S_j is an **exact optimal solution** to problem (**SSM**) w.r.t. some size constraint

With the aid of the result of Fujishige (1980), we can show that $S_j = T_j$ for all j , where each T_j is the subset returned by the algorithm **SSM**



Application to synthetic data

- Networks are randomly generated from the GENRMF generator
- For each randomly generated network, we considered
 - the size-constrained minimum cut problem 😞
 - the densest k-subgraph problem 😊

The number of subsets (= d) found by the algorithm **SSM**:

dataset 1 (Genrmf-long)

<i>n</i>	cut	dense
63	2	50
126	2	101
256	2	213
525	2	466
1008	2	868



dataset 2 (Genrmf-wide)

<i>n</i>	cut	dense
75	2	68
147	2	136
324	2	298
576	2	530
1024	2	975



problems exactly solved

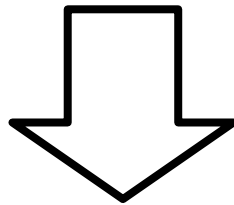
68 problems
are exactly
solved among
76 problems
(68/76=89%)

Application to real data

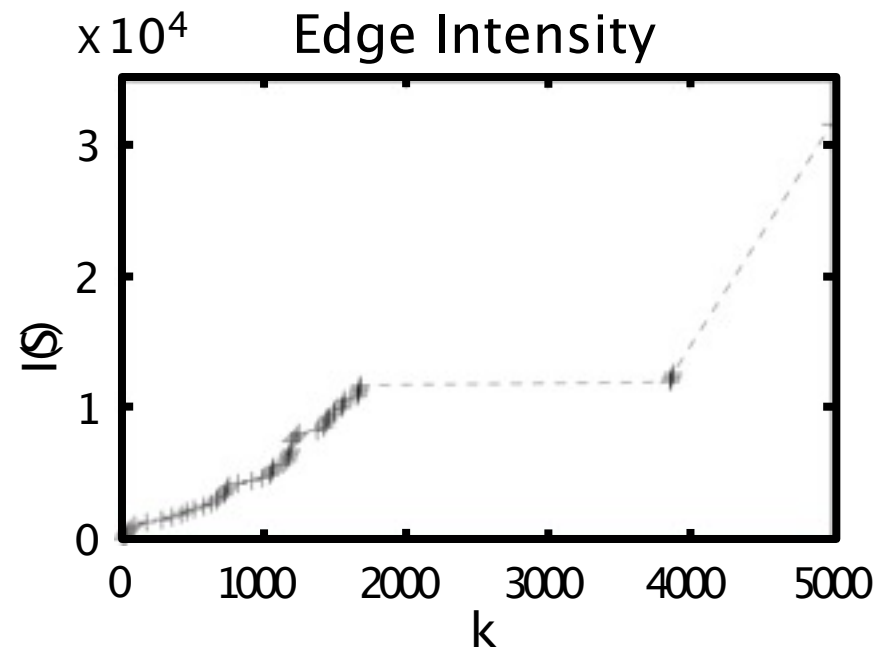
We applied the algorithm **SSM** to the densest k -subgraph problems on the network with **5,000** nodes and **31,664** edges ($n = 5000$)

This is a sub-network of social network data cnr-2000 (<http://law.dsi.unimi.it/webdata/cnr-2000>)

unweighted network



The algorithm provides optimal solutions for 57 out of 5000 size levels



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- Exact approach to size-constrained submodular minimization (Nagano-Kawahara-Aihara, ICML'11)
 - Example: Densest subgraph problem
 - Size-constrained submodular minimization (SSM)
 - The algorithm through the minimum norm base
- **Exact approach to clustering problems with submodular objective functions (Nagano-Kawahara-Iwata, NIPS'10)**
 - Example: Clustering of a network (minimum k-cut)
 - Minimum Average Cost (MAC) clustering
 - The algorithm using the Dilworth truncation
- Remarks

Clustering problems

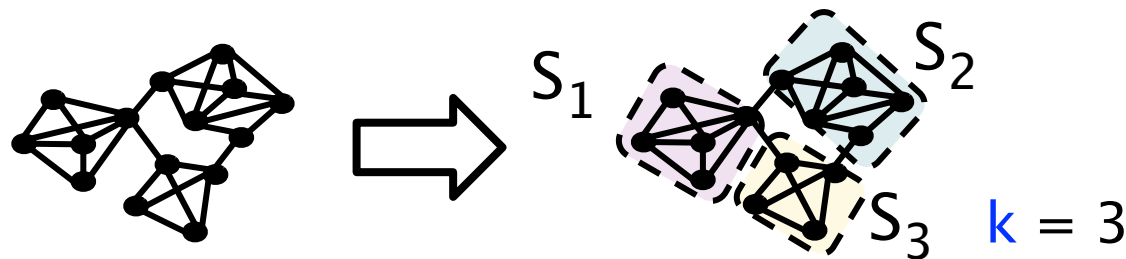
clusters

Given a set of data points $N = \{1, \dots, n\}$ and an integer $k \leq n$, find a partition of N into k subsets $S_1, \dots, S_k \neq \{\}$ (called clusters) such that points in the same cluster are similar to each other and points in different clusters are dissimilar

- In many cases, k is not given in advance

Clustering methods

k-means, spectral clustering, maximum margin, etc



Example: clustering of networks

Example: clustering of a network

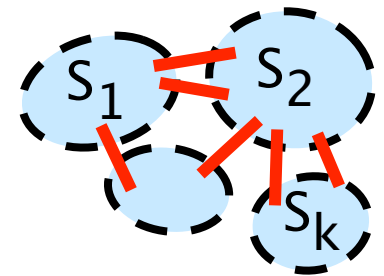
- Given a network $G = (N, E)$ with nonnegative edge weights
- Each edge indicates that its two endpoints are related

Find an “optimal” k -clustering

⇒ Compute a k -partition $\{S_1, \dots, S_k\}$ that minimizes

sum of weights of red edges = $\frac{1}{2} \sum_{i=1}^k C(S_i)$

⇒ minimum k -cut (NP-hard)



Objective function:

$$\sum_{i=1}^k C(S_i) \xrightarrow{\text{generalize}} \sum_{i=1}^k f(S_i) \quad \text{Narasimhan-Jojic-Bilmes, NIPS '05}$$

f is a general submodular function

Clustering with submodular functions

$f: 2^N \rightarrow \mathbf{R}$ is a general submodular function with $f(\{\}) = 0$

■ Optimal k -clustering problem [Narasimhan *et al.*, NIPS '05]

$$\begin{array}{ll} \min & \sum_{i=1}^k f(S_i) \\ \text{s. t.} & \{S_1, \dots, S_k\} \text{ is a } k\text{-partition of } N \end{array}$$

● k should be computed via some method

☹ NP-hard

➤ generalizes clustering problems with some natural criteria

Precisely speaking, they dealt with a symmetric submodular function f and their clustering method is based on the algorithm of Queyranne (1998)

We will change the objective function

$$\begin{array}{ccc} \sum_{i=1}^k f(S_i) & \Longrightarrow & \frac{\sum_{i=1}^k f(S_i)}{k-1} \\ k: \text{ fixed} & & k: \text{ not fixed} \end{array}$$

Clustering with submodular functions

$f: 2^N \rightarrow \mathbf{R}$ is a general submodular function with $f(\{\}) = 0$

■ Optimal k -clustering problem [Narasimhan *et al.*, NIPS '05]

$$\begin{array}{ll} \min & \sum_{i=1}^k f(S_i) \\ \text{s. t.} & \{S_1, \dots, S_k\} \text{ is a } k\text{-partition of } N \end{array}$$

● k should be computed via some method

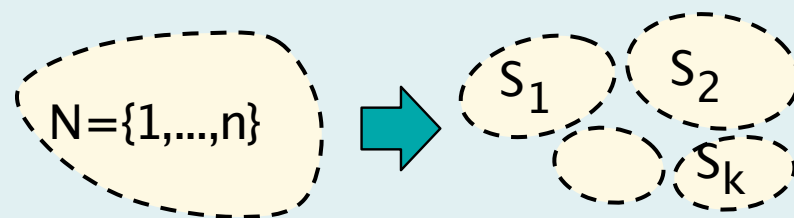
☹ NP-hard

■ Minimum Average Cost (MAC) clustering [This work]

$$\begin{array}{ll} \min & \sum_{S \in \mathcal{P}} f(S) / (|\mathcal{P}| - 1) \\ \text{s. t.} & \mathcal{P}^{S \in \mathcal{P}} \text{ is a partition of } N \\ & |\mathcal{P}| > 1 \end{array}$$

Generalization using a parameter $\beta \in [0, n]$

This is a natural **average cost function**



$$\begin{array}{ll} \text{cost: } 0 \rightarrow \sum_i f(S_i) & \left. \vphantom{\sum_i f(S_i)} \right\} \sum_i f(S_i) \\ \# \text{ of sets: } 1 \rightarrow k & \left. \vphantom{\sum_i f(S_i)} \right\} \frac{\sum_i f(S_i)}{k-1} \end{array}$$

Clustering with submodular functions

$f: 2^N \rightarrow \mathbf{R}$ is a general submodular function with $f(\{\}) = 0$

■ Optimal k -clustering problem [Narasimhan *et al.*, NIPS '05]

$$\begin{array}{ll} \min & \sum_{i=1}^k f(S_i) \\ \text{s. t.} & \{S_1, \dots, S_k\} \text{ is a } k\text{-partition of } N \end{array}$$

● k should be computed via some method

☹ NP-hard

■ Minimum Average Cost (MAC) clustering [This work]

$$\begin{array}{ll} \min & \sum_{S \in \mathcal{P}} f(S) / (|\mathcal{P}| - \beta) \\ \text{s. t.} & \mathcal{P} \text{ is a partition of } N \\ & |\mathcal{P}| > \beta \end{array}$$

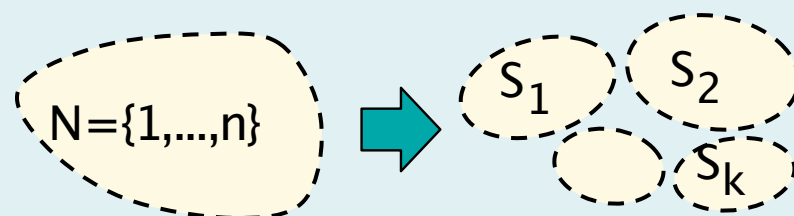
where $0 \leq \beta < n$

β - MAC clustering

If β is small, \mathcal{P} is coarse

If β is large, \mathcal{P} is fine

This is a natural **average cost function**



$$\begin{array}{ll} \text{cost: } 0 \rightarrow \sum_i f(S_i) & \left. \vphantom{\sum_i f(S_i)} \right\} \sum_i f(S_i) \\ \# \text{ of sets: } 1 \rightarrow k & \left. \vphantom{\sum_i f(S_i)} \right\} \frac{\sum_i f(S_i)}{k-1} \end{array}$$

Clustering with submodular functions

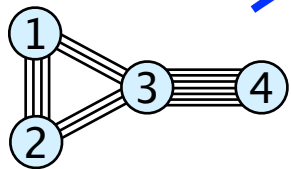
There is a relationship between the above two problems:

Prop. If a k -partition \mathcal{P} is a β -MAC clustering for some β , then \mathcal{P} is an optimal k -clustering

⇒ Information about MAC clusterings gives partial information about optimal k -clusterings

(Remember that an optimal k -clustering problem is NP-hard)

Example



Compute all β -MAC clusterings

$$0 \leq \beta < 1$$

$\{\{1, 2, 3, 4\}\}$
opt 1-clustering

$$1 \leq \beta < 11/7$$

$\{\{1\}, \{2\}, \{3, 4\}\}$
opt 3-clustering

$$11/7 \leq \beta < 4$$

$\{\{1\}, \{2\}, \{3\}, \{4\}\}$
opt 4-clustering

In this case, the MAC clustering algorithm computes optimal k -clusterings for $k = 1, 3, 4$

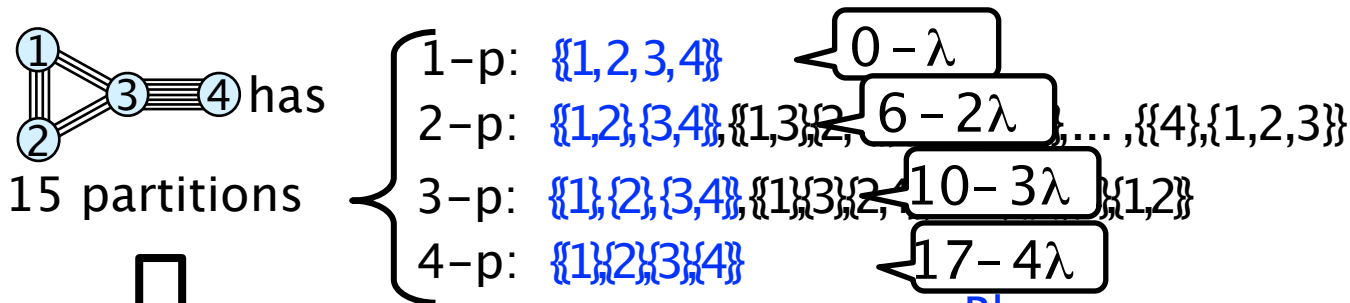
Let us see the framework of MAC clustering algorithm

Structure property of MAC clusterings (1/2)

Define a piecewise linear function $h : \mathbf{R}_+ \rightarrow \mathbf{R}$ as

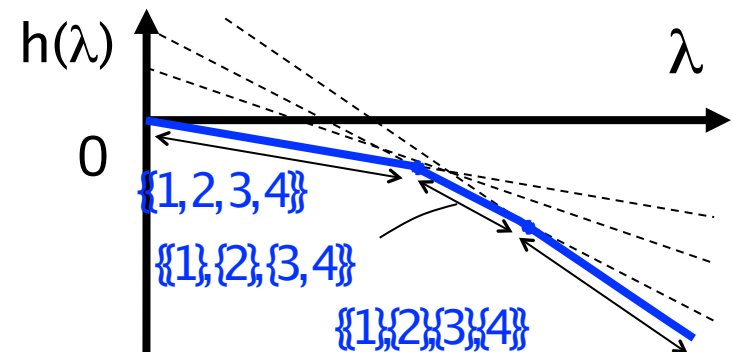
$$h(\lambda) = \min_{S \in \mathcal{P}} \{ \sum f(S) - |\mathcal{P}| \lambda : \mathcal{P} \text{ is a partition of } N \} \quad (\lambda \geq 0)$$

linear function in λ



$$h(\lambda) = \min \{-\lambda, 6-2\lambda, 10-3\lambda, 17-4\lambda\}$$

$\{1,2\}, \{3,4\}$ does not determine h



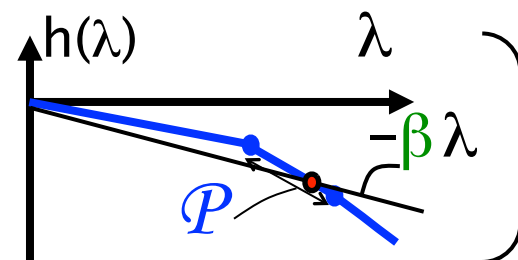
Structure property of MAC clusterings (2/2)

$$h(\lambda) = \min \left\{ \sum_{S \in \mathcal{P}} f(S) - |\mathcal{P}| \lambda : \mathcal{P} \text{ is a partition of } N \right\} (\lambda \geq 0)$$

linear function in λ

If we know the structure of h , for any $\beta \in [0, n)$, a β -MAC clustering can be found immediately.

For $\beta \in [0, n)$, a partition \mathcal{P} that corresponds to λ with $h(\lambda) = -\beta \lambda$ is a β -MAC clustering



Full information about the structure of the piecewise linear concave function h



Full information about all the β -MAC clusterings

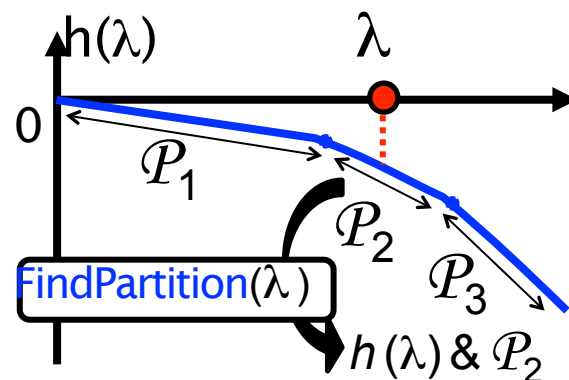
Framework of MAC clustering algorithm

(Full info about h) = (Partitions $\mathcal{P}_1, \dots, \mathcal{P}_d$ that determines h)

- The MAC algorithm uses

Procedure $\text{FindPartition}(\lambda)$:

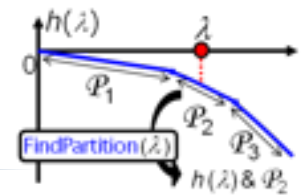
For $\lambda \geq 0$, the procedure computes $h(\lambda)$ & a partition \mathcal{P} that determines h at λ



With the aid of the Dilworth truncation, this procedure runs in $O(n \cdot \text{SFM}(n))$ time $\xrightarrow{\text{unconstrained submodular minimization}}$

- By performing FindPartition $O(n)$ times, we obtain all \mathcal{P}_j

Theorem [This work] Full information about all β -MAC clusterings can be computed in $O(n^2 \cdot \text{SFM}(n))$ time



Procedure FindPartition(λ)

This procedure solves

$$\begin{aligned} h(\lambda) = \min_{S \in \mathcal{P}} \sum (f(S) - \lambda) \\ \text{s.t. } \mathcal{P} \text{ is a partition of } N \end{aligned}$$

Define $f^\lambda: 2^N \rightarrow \mathbf{R}$ as $f^\lambda(S) = \begin{cases} f(S) - \lambda & \text{if } S \text{ is nonempty} \\ 0 & \text{if } S \text{ is empty} \end{cases}$

➡ f^λ is an intersecting submodular function

Let $f_p^\lambda: 2^N \rightarrow \mathbf{R}$ be the **Dilworth truncation** (1944) of f^λ

$$\left[f_p^\lambda(S) = \min \left\{ \sum_{S \in \mathcal{P}} f^\lambda(S) : \mathcal{P} \text{ is a partition of } S \right\} \right]$$

➡ Then, $h(\lambda) = f_p^\lambda(N) = \min \left\{ \sum_{S \in \mathcal{P}} f^\lambda(S) : \mathcal{P} \text{ is a partition of } N \right\}$

An optimal partition can be found in $O(n \cdot \text{SFM}(n))$ time

See Chapter 48 of Schrijver's book [2003]

Experimental results

We compared the **MAC** algorithm with

- (1) k-means method
- (2) spectral-clustering method with normalized-cut (Ng+, 2002)
- (3) maximum-margin clustering (Xu+, 2005)

of clusters k is selected through 5-fold cross-validation

	Gaussian	Circle	Iris	Libras	Glass	360 samples
k-means	1.0	0.88	0.79	0.85	0.93	'Gaussian', 'Circle': synthetic datasets
norm cut	0.88	0.86	0.84	0.87	0.93	
max margin	0.99	1.0	0.96	0.90	0.97	'Iris', 'Libras', 'Glass': real world datasets from the UCI repository
MAC	0.99	1.0	0.99	0.97	0.97	

Clustering accuracy (the larger, the better)

MAC clustering is competitive with standard clustering methods

Remarks

- Submodular optimization problems are extensively studied in machine learning
- The proposed algorithms run in polynomial time
- The results contrast sharply with the NP-hardness of the problems
- Minimization of the difference of two submodular functions is also an important problem in ML

$$\min_{S \subseteq N} f_1(S) - f_2(S)$$

↖ Discrete version
of DC programming

Narasimhan-Bilmes (UAI'05),
Kawahara-Washio (NIPS '11)

END

Appendix: Description of FindPartition

$V = \{1, \dots, n\}$, $V^m = \{1, \dots, m\}$ for each $m = 1, \dots, n$

\mathbf{e}_m is the m -th unit vector $\in \mathbf{R}^n$ for each $m = 1, \dots, n$

Procedure FindPartition (λ)

Input: A real value $\lambda \geq 0$

Output: A real value $h(\lambda)$ and a partition \mathcal{P}_λ of V

S1: Set $\mathcal{P}^0 := \{\}$.

Set $\mathbf{x}^0 := -M \cdot \mathbf{1}_n = (-M, \dots, -M)$ for some large $M > 0$.

S2: For each $m = 1, \dots, n$, do

Compute $\alpha^m = \min \{ f(S) - \mathbf{x}^{m-1}(S) - \lambda : m \in \forall S \subseteq V^m \}$
and $T^m = \operatorname{argmin} \{ f(S) - \mathbf{x}^{m-1}(S) - \lambda : m \in \forall S \subseteq V^m \}$.



Set $\mathbf{x}^m := \mathbf{x}^{m-1} + \alpha^m \cdot \mathbf{e}_m$,
set $U^m := T^m \cup [\cup \{S : S \in \mathcal{P}^{m-1}, T^m \cap S \neq \{\}\}]$, and
set $\mathcal{P}^m := \{U^m\} \cup \{S : S \in \mathcal{P}^{m-1}, T^m \cap S = \{\}\}$.

S3: Return $h_\lambda := \mathbf{x}^n(V)$ and $\mathcal{P}_\lambda := \mathcal{P}^n$.
